

Surface deformation caused by the Abrikosov vortex lattice

Pavel Lipavský^{1,4}, Klaus Morawetz^{2,3}, Jan Koláček⁴ and Ernst Helmut Brandt⁵

¹ Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

² Forschungszentrum Rossendorf, PF 51 01 19, 01314 Dresden, Germany

³ Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, 01187 Dresden, Germany

⁴ Institute of Physics, Academy of Sciences, Cukrovarnická 10, 16253 Prague 6, Czech Republic and

⁵ Max Planck Institute for Metals Research, D-70506 Stuttgart, Germany

In superconductors penetrated by Abrikosov vortices the magnetic pressure and the inhomogeneous condensate density induce a deformation of the ionic lattice. We calculate how this deformation corrugates the surface of a semi-infinite sample. The effect of the surface dipole is included.

PACS numbers: 74.20.De, 74.25.Ld, 74.25.Qt, 74.81.-g

I. INTRODUCTION

Deformations of the ionic lattice caused by the Abrikosov vortices have been studied from several aspects. For example, if a vortex moves, the motion of such deformation demands a motion of ions which contributes to the inertial mass of the vortex.^{1,2,3} In the static case, forces evoked by vortices create a tension which modifies the total volume of the sample and which was observed as magnetostriction.⁴ Moreover, in anisotropic materials the elastic energy caused by vortices depends on the relative orientation of the Abrikosov vortex lattice and the crystal lattice.^{5,6}

In the above mentioned studies a vortex was treated as infinitely long. This idealized geometry essentially simplifies the problem. Since the system has translational symmetry along the vortex line, the lattice deformation is purely longitudinal with the displacement vectors perpendicular to the vortex.^{1,4}

As far as we know, nobody has studied deformations near the surface, where the magnetic flux of the vortex leaves the superconductor. In the present paper we focus on this problem. For simplicity we assume that the sample is semi-infinite and the applied magnetic field is perpendicular to its surface, see figure 1.

Far from the surface the lattice deformation approaches its bulk value with displacement vectors perpendicular to vortices, i.e., parallel to the surface. Let us sketch in advance which complications one can expect near the surface.

As seen in figure 1, the stretching magnetic field together with circulating currents result in a Lorentz force with a component pointing along the vortex. Electric fields balancing this force act also on the ion lattice and corrugate the surface.

Beside the Lorentz force, one can imagine two additional mechanisms leading to the corrugation. First, the specific volume of the superconducting and normal states differ. The normal metal in the vortex core is pulled by its neighborhood to adopt the specific volume of the superconductor. As mentioned above, deep in the bulk these stresses cause displacements perpendicular to the vortex. Close to the surface, however, the same stresses

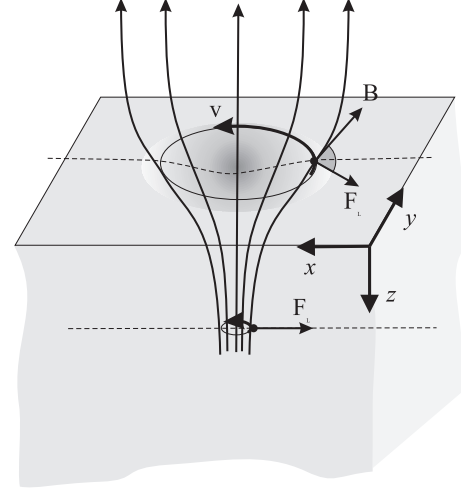


FIG. 1: Lorentz force acting on the circulating superconducting current. In the bulk the Lorentz force is parallel to the surface. Near the surface it is not parallel due to the magnetic stray field.

lead to different deformations as they are partially relaxed by displacements perpendicular to the surface, i.e., along the vortex.

Second, the surface dipole which confines the electrons in the crystal changes under transition from the normal to the superconducting state. Accordingly, at the vortex core the surface dipole differs from other regions of the surface. The force which holds electrons inward naturally pulls the oppositely charged ions outwards and also corrugates the surface. The general relation between the surface dipole and the surface tension has been established already two decades ago.^{7,8} The contribution of the superconducting condensate has been discussed only recently.⁹

The paper is organized as follows. In sections II and III we introduce the basic set of equations for elastic deformations of an isotropic material near the surface. The surface deformation due to the Abrikosov vortex lattices is discussed in section IV and the numerical solutions for Nb and YBa₂Cu₃O₇ are presented in section V. Section VI with the conclusions ends the paper.

II. ELASTIC DEFORMATIONS IN ISOTROPIC MEDIUM

In this section we recall the basic definitions needed to describe the elastic deformations of an isotropic medium. More details the reader can find in the textbook of Landau and Lifshitz.¹⁰

A. Tensors of strain and stress

Deformations are described by atomic displacements \mathbf{u} . We assume that all atoms are identical and only a single atom occupies the elementary cell. Since the interatomic distance is short compared to the characteristic scales of deformations, we treat $\mathbf{u}(x, y, z)$ as a function of continuous coordinates.

The space derivatives of the displacement define the strain tensor. For small deformations assumed here its components read

$$u_{xy} = \frac{1}{2} \left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right). \quad (1)$$

The complementary anti-symmetric combination of derivatives corresponds to the rotation of the rigid body, therefore it does not contribute to deformations.

The strain creates a stress described by a tensor σ . In general $\sigma_{\kappa\tau} = \sum_{\mu\nu} \Lambda_{\kappa\tau\mu\nu} u_{\mu\nu}$, where Λ is 4th order tensor of elastic coefficients. The Greek indices stand for x, y, z . For an isotropic medium this relation simplifies to

$$\sigma_{\kappa\tau} = K(\nabla \cdot \mathbf{u}) \delta_{\kappa\tau} + 2\mu \left(u_{\kappa\tau} - \frac{1}{3}(\nabla \cdot \mathbf{u}) \delta_{\kappa\tau} \right), \quad (2)$$

where the divergence of the displacement vector

$$(\nabla \cdot \mathbf{u}) = u_{xx} + u_{yy} + u_{zz} \quad (3)$$

is a shorthand notation for the trace of the strain tensor. It represents the local change of the specific volume. The tensor $u_{\kappa\tau} - \frac{1}{3}(\nabla \cdot \mathbf{u}) \delta_{\kappa\tau}$ has zero trace and describes purely shear deformations. The coefficients K and μ are called the bulk and shear modulus, respectively.

B. Stability conditions

The stress depends on local gradients of the displacements, i.e., on changes of the bond lengths between neighboring atoms. Accordingly it represents only contact forces while long-range forces have to be covered separately. Here we shall consider a non-contact force due to interaction of the crystal lattice with superconducting electrons.

The gradient of the stress balances a long-range force \mathbf{F} acting on a unitary volume $\sum_{\kappa} \nabla_{\kappa} \sigma_{\kappa\tau} + F_{\tau} = 0$, where

$\nabla_x \equiv \frac{\partial}{\partial x}$ and so on. For the isotropic material this stability condition reads¹⁰

$$\left(K + \frac{4}{3}\mu \right) \nabla(\nabla \cdot \mathbf{u}) - \mu [\nabla \times [\nabla \times \mathbf{u}]] = \mathbf{F}. \quad (4)$$

In this paper we consider forces that can be expressed as a gradient of the potential U

$$\mathbf{F} = -\nabla U. \quad (5)$$

In our numerical studies below we assume that this potential is exclusively due to the electrostatic potential φ acting on the charge density of the ionic lattice ρ , i.e., $U = \rho\varphi$.

Alternatively, one can assume an effective potential $U = 2K\alpha_0|\psi|^2/n$ corresponding to the force used by Šimánek and Duan^{1,2} and Coffey⁴. Here α_0 is the relative volume difference between the superconducting and the normal states, K is the bulk modulus, ψ is the Ginzburg-Landau (GL) wave function and n is the density of pairable electrons.

These two choices of the potential U yield very similar results. They are not completely identical, however. For example, the electrostatic potential known as the Bernoulli potential covers the Lorentz force, while the effective potential $U = 2K\alpha_0|\psi|^2/n$ does not.¹¹

C. Surface conditions

At the surface the balance of forces demands $\sum_{\kappa} n_{\kappa} \sigma_{\kappa\tau} + P_{\tau} = 0$, where \mathbf{n} is a unit vector normal to the surface and \mathbf{P} is the external force on a unit area of the surface. The normal component $p = (\mathbf{n} \cdot \mathbf{P})$ is the pressure. We will not assume tangential surface forces in this paper.

To simplify boundary conditions we specify the geometry of our sample. It is a semi-infinite superconductor in the half-space $z > 0$. For the normal vector $\mathbf{n} = (0, 0, -1)$ and normal surface force $\mathbf{P} = (0, 0, -p)$ we find three surface conditions

$$\begin{pmatrix} \sigma_{xz} \\ \sigma_{yz} \\ \sigma_{zz} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -p \end{pmatrix}. \quad (6)$$

Using the linear relation between stress and strain, the surface conditions (6) are converted into conditions for the displacement \mathbf{u} . For the isotropic medium from (2) and (6) follows

$$\begin{aligned} u_{xz} &= 0, \\ u_{yz} &= 0, \\ \left(K + \frac{4}{3}\mu \right) u_{zz} + \left(K - \frac{2}{3}\mu \right) (u_{xx} + u_{yy}) &= -p. \end{aligned} \quad (7)$$

The pressure p includes the ambient pressure of coolant which is homogeneous all over the sample surface. We ignore it, because it does not contribute to the corrugation.

We do not want to list all possible forces acting on the surface. We merely mention that the surface of the sample feels the surface dipole $\delta\varphi$, which acts as an effective pressure $p = -\rho\delta\varphi$, see Ref. 9. The dipole amplitude $\delta\varphi = \varphi(0) - \varphi(\infty)$ is the difference between the electrostatic potential at the surface and deep in the bulk of the superconductor. The surface dipole is conveniently evaluated from the GL free energy with the help of the Budd-Vannimenus theorem^{12,13} adopted to superconductor^{9,14}.

Now the problem is fully specified. The displacement \mathbf{u} is driven by the potential U and the effective pressure p . These quantities can be treated within any approximation the reader prefers. In section V we will relate them to the electrostatic potential φ and the surface dipole $\delta\varphi$. At the moment we merely assume that the potential and the pressure are known functions of the GL wave function. Since the deformation has only a negligible effect on the GL wave function, the GL wave function obtained from the ordinary GL theory can be used. We take the GL wave function as known and focus on the deformation.

III. INDUCED AND FREE DEFORMATION

As mentioned in the introduction, the deformation near the surface has three sources – magnetic stray field, expansion or contraction along the vortex, and the surface dipole. Since the elastic equation (4) and its boundary conditions (7) are linear in \mathbf{u} , it is possible to separate individual contributions.

As the first step, it is advantageous to separate the displacement \mathbf{u} into two parts – induced deformation \mathbf{u}^i driven by the long range force \mathbf{F} which induces displacements all over the sample, and the free deformation \mathbf{u}^f . So we write

$$\mathbf{u} = \mathbf{u}^i + \mathbf{u}^f, \quad (8)$$

where the displacement \mathbf{u}^i is longitudinal

$$[\nabla \times \mathbf{u}^i] = 0. \quad (9)$$

and obeys the equation

$$\left(K + \frac{4}{3}\mu\right) (\nabla \cdot \mathbf{u}^i) = -U(\mathbf{r}, z). \quad (10)$$

Since the differential equation (10) is of the first order, this induced displacement is fully specified by the potential U and the requirement of convergence deep in the sample.

After substitution of (8) into the elastic equation (4), the stress from the induced displacement compensates the long range forces and one is left with the equation for the free displacement

$$\left(K + \frac{4}{3}\mu\right) \nabla(\nabla \cdot \mathbf{u}^f) - \mu [\nabla \times [\nabla \times \mathbf{u}^f]] = 0. \quad (11)$$

This is a second-order differential equation and we need to find the solution which in addition to the convergence deep inside guarantees also the fulfillment of the surface boundary condition.

A. Laplace equation for the free deformation

Now we show that it is possible to simplify equation (11) to the Laplace equation.

Taking the divergence of equation (11) we find that

$$\nabla \cdot (\nabla^2 \mathbf{u}^f) = 0, \quad (12)$$

because the divergence of a rotation is zero. Taking the rotation of equation (11) we find

$$[\nabla \times (\nabla^2 \mathbf{u}^f)] = 0, \quad (13)$$

because the rotation of a gradient is also zero. The vector identity $[\nabla \times [\nabla \times \mathbf{u}^f]] = \nabla(\nabla \cdot \mathbf{u}^f) - \nabla^2 \mathbf{u}^f$ was used in the rearrangement.

According to (12) and (13) all the derivatives of $\nabla^2 \mathbf{u}^f$ are zero, therefore it is a constant. A finite value of \mathbf{u}^f for $z \rightarrow \infty$ is possible only if this constant is zero. We thus have

$$\nabla^2 \mathbf{u}^f = 0. \quad (14)$$

Being free of material parameters, this Laplace equation is more convenient than the equation (11).

B. Surface matching

The surface boundary condition (7) applies to the total displacement. Substituting (8) into (7) we obtain

$$\begin{aligned} u_{xz}^f &= -u_{xz}^i, \\ u_{yz}^f &= -u_{yz}^i, \\ \left(K + \frac{4}{3}\mu\right) u_{zz}^f + \left(K - \frac{2}{3}\mu\right) (u_{xx}^f + u_{yy}^f) \\ &= -p - \left(K + \frac{4}{3}\mu\right) u_{zz}^i - \left(K - \frac{2}{3}\mu\right) (u_{xx}^i + u_{yy}^i). \end{aligned} \quad (15)$$

These conditions determine gradients of \mathbf{u}^f at $z = 0$. The induced deformation \mathbf{u}^i is already known, therefore we have moved its strain elements to the right hand sides of the boundary conditions.

By conditions (15) the free displacement is fully specified. The second boundary condition is the request of convergency, $u^f \rightarrow 0$ for $z \rightarrow \infty$. Now the set of equations is complete and we are ready to solve for the corrugation of the surface around the vortex ends.

IV. VORTEX LATTICE

If the vortices form an Abrikosov lattice, we can benefit from its periodic structure. In this case all components

of the displacement can be solved analytically in the two-dimensional (2D) Fourier representation.

A. Induced deformation

In the x - y plane, the potential is a sum of planar waves

$$U(\mathbf{r}, z) = \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} U(\mathbf{k}, z), \quad (16)$$

where $\mathbf{r} \equiv (x, y)$ is a 2D coordinate. The 2D wave vectors $\mathbf{k} = (k_x, k_y)$ attain discrete values given by the density of vortices and the actual structure of the Abrikosov lattice.

To solve the equation for the displacement requires some intermediate steps. Since the induced displacement \mathbf{u}^i is longitudinal, it can be expressed as the gradient of a scalar function

$$\mathbf{u}^i = \nabla \chi(\mathbf{r}, z). \quad (17)$$

In the 2D Fourier representation the equation (10) yields

$$\left(K + \frac{4}{3}\mu\right) \left(k^2 - \frac{\partial^2}{\partial z^2}\right) \chi = U(\mathbf{k}, z), \quad (18)$$

where $k^2 = k_x^2 + k_y^2$. It is solved by

$$\chi(\mathbf{k}, z) = \frac{1}{2k} \frac{1}{K + \frac{4}{3}\mu} \int_0^\infty dz' e^{-k|z-z'|} U(\mathbf{k}, z'). \quad (19)$$

We are interested namely in values at the surface

$$\chi(\mathbf{k}, 0) = \frac{1}{2k} \frac{1}{K + \frac{4}{3}\mu} \int_0^\infty dz' e^{-kz'} U(\mathbf{k}, z'). \quad (20)$$

The z -gradient at the surface follows from (19) as

$$u_z^i = \left. \frac{\partial}{\partial z} \chi(\mathbf{k}, z) \right|_{z=0} = k \chi(\mathbf{k}, 0). \quad (21)$$

The surface value of this displacement contributes to the surface corrugation.

The surface strain given by the second gradient follows from the equation (18) as

$$u_{zz}^i = \left. \frac{\partial^2}{\partial z^2} \chi(\mathbf{k}, z) \right|_{z=0} = k^2 \chi(\mathbf{k}, 0) - \frac{1}{K + \frac{4}{3}\mu} U(\mathbf{k}, 0). \quad (22)$$

This surface strain enters the boundary condition, where it serves as the source of the free deformation.

B. Free deformation

The free deviation \mathbf{u}^f has the same periodicity as the Abrikosov vortex lattice. From the Laplace equation (14) thus follows

$$\mathbf{u}^f(\mathbf{k}, z) = \mathbf{u}^f(\mathbf{k}, 0) e^{-kz}. \quad (23)$$

The boundary conditions (15) in the 2D Fourier representation read

$$\begin{aligned} \frac{1}{2}(ik_x u_z^f - k u_x^f) &= -ik_x k \chi(\mathbf{k}, 0), \\ \frac{1}{2}(ik_y u_z^f - k u_y^f) &= -ik_y k \chi(\mathbf{k}, 0), \\ -k \left(K + \frac{4}{3}\mu\right) u_z^f + \left(K - \frac{2}{3}\mu\right) (ik_x u_x^f + ik_y u_y^f) &= -p - 2\mu k^2 \chi(\mathbf{k}, 0) + U(\mathbf{k}, 0). \end{aligned} \quad (24)$$

We have used equation (23) to evaluate the derivatives on the left hand sides of (15) and the ansatz (17) together with relations (20-22) in the right hand sides of (15).

From the first and second conditions of (24) one eliminates u_x^f and u_y^f obtaining $ik_x u_x^f + ik_y u_y^f = -k u_z^f - 2k^2 \chi$. Using this relation in the third condition of (24) one arrives at the z -component of the free displacement

$$u_z^f = \frac{p - U(\mathbf{k}, 0) - 2k^2 \left(K - \frac{5}{3}\mu\right) \chi(\mathbf{k}, 0)}{2k \left(K + \frac{1}{3}\mu\right)}. \quad (25)$$

With u_z^f from (25) and the first and the second equations of (24) one readily evaluates the parallel displacements u_x^f and u_y^f , respectively. Here we want to concentrate on the component u_z^f perpendicular to the surface.

C. Surface corrugation

The corrugation of the surface is given by the total displacement in the z -direction $u_z = u_z^f + u_z^i$. Adding formulas (25) and (21) we obtain

$$\begin{aligned} u_z(\mathbf{k}) &= \frac{p - U(\mathbf{k}, 0) + 4k^2 \mu \chi(\mathbf{k}, 0)}{2k \left(K + \frac{1}{3}\mu\right)} \\ u_z(\mathbf{r}) &= \sum_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} u_z(\mathbf{k}). \end{aligned} \quad (26)$$

Formula (26) is the final result of the general part of our discussion. It provides the 2D Fourier decomposition of atomic displacements at the surface layer. In our notation a positive displacement u_z corresponds to the atomic motion inwards the superconductor.

V. NUMERICAL RESULTS FOR THE ELECTROSTATIC INTERACTION

To proceed we assume that the interaction between the super-electrons and the ionic lattice is exclusively carried by the mean electrostatic field. This approximation neglects the effect of the lattice density on the electronic band structure and on the phonon band structure and for many materials it might lead to quantitatively incorrect predictions. In this paper we adopt this approximation for its simplicity.

A. Surface dipole

As mentioned in the introduction, in the electrostatic approximation, the effective potential is proportional to the electrostatic Bernoulli potential φ , i.e.,

$$U(\mathbf{r}, z) = \rho\varphi(\mathbf{r}, z). \quad (27)$$

The Bernoulli potential is a function of the GL function¹⁵

$$e\varphi = -\frac{\partial\alpha}{\partial n}|\psi|^2 - \frac{1}{2}\frac{\partial\beta}{\partial n}|\psi|^4, \quad (28)$$

where $\alpha = \gamma(T^2 - T_c^2)/2n$ and $\beta = \gamma T^2/2n^2$ are the GL parameters expressed in terms of Sommerfeld's gamma. These values follow from the Gorter-Casimir two-fluid model in the limit $T \rightarrow T_c$, see Ref. 16. One can also use the limiting BCS values of α and β which are larger by factors 1.43 and 2.86 than the two-fluid limit, respectively.⁹

The pressure at the surface is caused by the surface dipole⁹

$$p(\mathbf{r}) = \rho\varphi_+(\mathbf{r}) - \rho\varphi_-(\mathbf{r}), \quad (29)$$

where $\varphi_{\pm}(\mathbf{r}) = \varphi(\mathbf{r}, \pm\epsilon)$ with $\epsilon > 0$ being an infinitesimal distance. In reality, ϵ has to exceed the Thomas-Fermi screening length and the BCS coherence length. The potential φ_+ is the extrapolation of the internal potential towards the surface, and φ_- represents the potential out of the crystal.

The surface value of the effective potential is defined as a limit from inside, therefore

$$U(\mathbf{r}, 0) \equiv \lim_{\epsilon \rightarrow 0} U(\mathbf{r}, \epsilon) = \rho\varphi_+(\mathbf{r}). \quad (30)$$

The displacement of the surface atoms (26) for the electrostatic approximation reads

$$u_z = -\frac{\rho}{2k(K + \frac{1}{3}\mu)}\varphi_-(\mathbf{k}) + \frac{2k\mu}{K + \frac{1}{3}\mu}\chi(\mathbf{k}, 0). \quad (31)$$

As one can see, the potential φ_+ cancels and we are left with the potential φ_- . According to the Budd-Vannimenus theorem for superconductors, the potential above the surface is proportional to the density of the free energy,^{14,17}

$$e\varphi_- = -\frac{\alpha}{n}|\psi|^2 - \frac{1}{2}\frac{\beta}{n}|\psi|^4, \quad (32)$$

which one conveniently evaluates within the Ginzburg-Landau theory. For details of the Bernoulli potential and the surface dipole see textbook [16].

B. Bulk forces

The internal value of the Bernoulli potential contributes only via the subsidiary function χ . In general

	$\frac{\gamma T_c^2}{4n}$ [μeV]	κ	n [10^{28}m^{-3}]	$\frac{\partial \ln T_c}{\partial \ln n}$	$\frac{\partial \ln \gamma}{\partial \ln n}$	E [GPa]	σ
Nb	4.585	1.5	2.2	0.74^{16}	0.42^{16}	105^{19}	0.4^{19}
YBCO	750	65	0.5	-4.82^{20}	-4.13^{20}	$200^{21,22}$	0.2^{22}

TABLE I: Material parameters of Niobium and $\text{YBa}_2\text{Cu}_3\text{O}_7$: condensation energy per particle, GL parameter, particle density and logarithmic derivatives of the critical temperature and the linear coefficient of the specific heat γ , Young's modulus and Poisson ratio.

one needs the complete 3D solution of the vortex lattice near the surface. Numerical studies have shown that one can neglect the z dependence of the amplitude of the GL function everywhere including the close vicinity of the surface.¹⁸ The amplitude variation is about 1%. Since the Bernoulli potential depends exclusively on the amplitude of the GL function, the potential has the same value as deep in the bulk, $\varphi(\mathbf{r}, z) \approx \varphi_{\infty}(\mathbf{r})$, for any z .

Neglecting the z dependence of the potential, the integral in (20) becomes trivial giving

$$\chi(\mathbf{k}, 0) = \frac{1}{2k^2} \frac{\rho}{K + \frac{4}{3}\mu} \varphi_{\infty}(\mathbf{k}). \quad (33)$$

The potential φ_{∞} is conveniently found from (28) using the GL function deep in the sample. For a fixed magnetic field, the GL function deep in the sample is the same as in the infinite sample, therefore it can be evaluated as an effectively two-dimensional problem.

C. Surface corrugation

The displacement of the surface atoms results from (31) and (33) as

$$u_z = -\frac{\rho}{2k(K + \frac{1}{3}\mu)} \left[\varphi_-(\mathbf{k}) - \frac{2\mu}{K + \frac{4}{3}\mu} \varphi_{\infty}(\mathbf{k}) \right]. \quad (34)$$

One can see from (34) that the relative contribution of the bulk and the surface potentials depends on the shear modulus μ . For soft materials with $\mu \ll K$ the bulk potential gives a negligible contribution so that the surface corrugation is driven only by the electrostatic potential above the surface. In this case the corrugation is independent of the density derivatives of the GL parameters.

Many authors dealing with deformable superconductors prefer to express elastic coefficients via the Poisson ratio $\sigma = (K - \frac{2}{3}\mu) / (2K + \frac{2}{3}\mu)$ and the Young modulus $E = 3K(1 - 2\sigma)$. In this notation the displacement of surface atoms (34) reads

$$u_z = \frac{(1 - 2\sigma)(1 + \sigma)}{kE(1 - \sigma)} \{ (1 - \sigma)p(\mathbf{k}) - \rho\sigma\varphi_{\infty}(\mathbf{k}) \}. \quad (35)$$

Deriving (35) we have used that the Bernoulli potential is nearly independent of z so that $\varphi_+ = \varphi_{\infty}$. The pressure at the surface (29) thus equals $p = \rho(\varphi_{\infty} - \varphi_-)$.

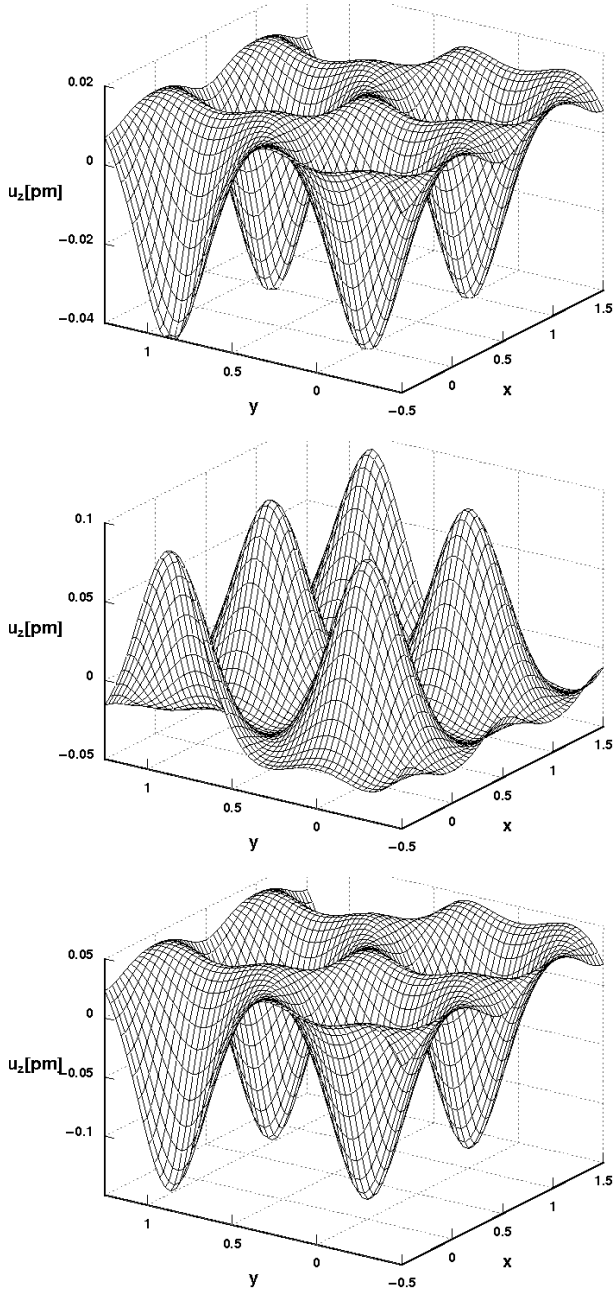


FIG. 2: Surface corrugation $u_z(\mathbf{r})$ of Nb (above) compared with the value neglecting surface dipoles (middle) and only surface dipoles (below). The temperature and the mean magnetic field are $T = 0.95 T_c = 9$ K and $\bar{B} = 0.21 B_{c2}(T) = 6.4$ mT. Length unit is the vortex distance $a = 128$ nm.

The numerical study of the surface corrugation (35) is performed with the parameters listed in the table I. Figure 2 presents the surface corrugation of Niobium with the GL parameters κ increased by impurities to 1.5. The scale is in $\text{pm} = 10^{-2} \text{ \AA}$, therefore the maximum deformation $\sim 5 \cdot 10^{-4} \text{ \AA}$ is far too small to be detected by recent scanning microscopes. In our convention the negative u_z corresponds to atoms displaced out of the crystal.

The total deviation of atoms at the surface is seen in

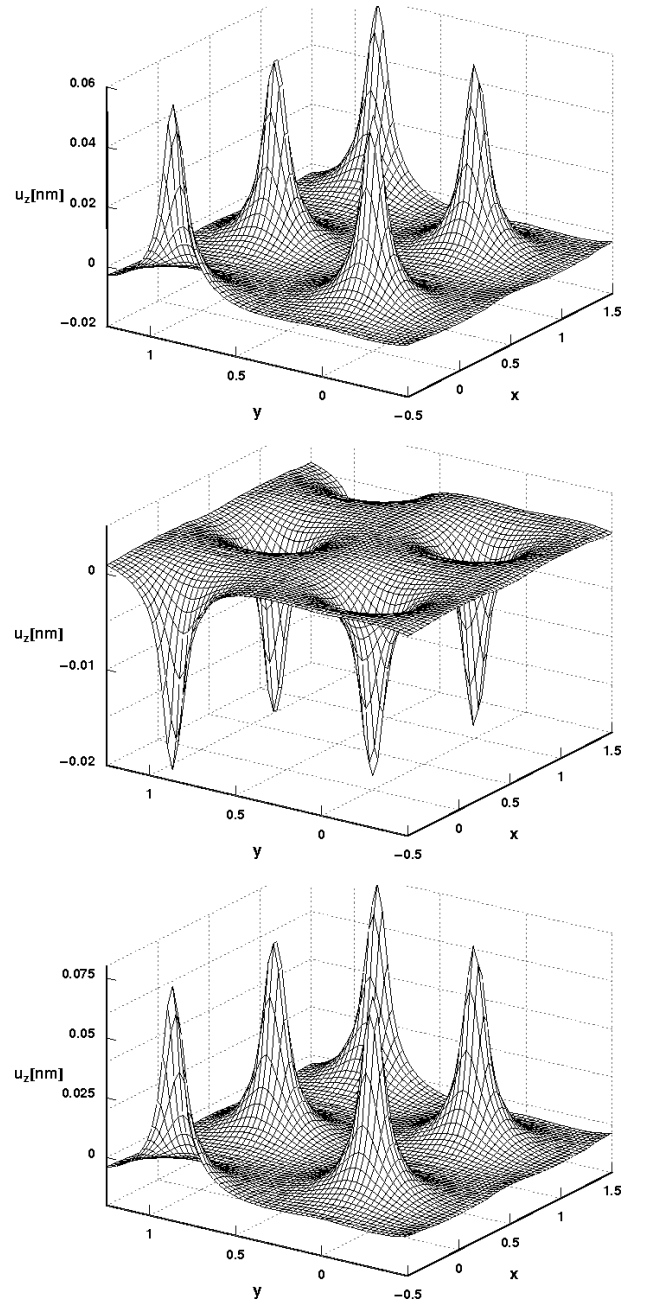


FIG. 3: Surface corrugation $u_z(\mathbf{r})$ of $\text{YBa}_2\text{Cu}_3\text{O}_7$ (above) compared with the value neglecting surface dipoles (middle) and only surface dipoles (below). The temperature and the mean magnetic field are $T = 0.67 T_c = 60$ K and $\bar{B} = 0.01 B_{c2}(T) = 0.6$ T. Length unit is the vortex distance $a = 58$ nm.

the upper part of figure 2. The middle part shows the deviation evaluated omitting the surface dipole, i.e., setting $p = 0$ in formula (35). As one can see, such approximation for Niobium leads to the opposite sign of the atomic displacement. The lower part shows the surface deformation evaluated from the surface dipole only. This approximation overestimates the amplitude more than twice.

The magnitude of the surface corrugation is directly proportional to the condensation energy per particle, which for Niobium has the value $\frac{\gamma T_c^2}{4n} = 4.6 \mu\text{eV}$. In conventional superconductors this condensation energy per particle is small because of the small critical temperature, $T_c = 9.5$ K and the large density of particles, $n = 2.2 \cdot 10^{28}/\text{m}^3$.

In high- T_c superconductors the critical temperature is larger by a factor of ten, while the density of particles is lower by a factor of ten. This leads to an appreciably larger condensation energy per particle. For example, in $\text{YBa}_2\text{Cu}_3\text{O}_7$ one has $T_c = 90$ K and $n = 5 \times 10^{27} \text{ m}^{-3}$ resulting into $\frac{\gamma T_c^2}{4n} = 750 \mu\text{eV}$. Figure 3 presents a corrugation of the $\text{YBa}_2\text{Cu}_3\text{O}_7$ surface with the surface parallel to the a - b planes, i.e., the magnetic field along the c axis. As one can see, the maximum displacement of the surface atom is more than 0.5 \AA , which can be observed by the scanning microscope. Again, neglecting the surface dipole one arrives at the opposite displacements, while using only the surface dipole one overestimates the magnitude.

Perhaps we should note that application of the isotropic model to the layered structure of $\text{YBa}_2\text{Cu}_3\text{O}_7$ is not justified. One clearly needs more elastic coefficients to describe the deformation of this highly anisotropic material.²³ The presented data can thus serve only as an order of magnitude estimate.

VI. CONCLUSIONS

Magnetic field entering the superconductor in the form of vortices induces a corrugation of the surface. In conventional superconductors the displacement of surface atoms is of the order of 10^{-4} \AA , which is too small to be observed by recent experimental tools. In high- T_c superconductors one can expect amplitudes $\sim 10^{-1} \text{ \AA}$ which is in the reach of scanning force microscopes.

Our results for Niobium and $\text{YBa}_2\text{Cu}_3\text{O}_7$ show that among the forces that drive the surface corrugation the dominant one is due to the surface dipole. The contribution of the bulk potential to the surface corrugation is opposite to the contribution of the surface, therefore it reduces the magnitude of the atomic displacement.

Since the deformation of the crystal near the surface differs from the deformation in the bulk, one can expect that the surface terms play an important role in the Šimánek contribution to the vortex mass in thin layers. We leave this problem for a future work.

This work was supported by research plans MSM 0021620834 and No. AVOZ10100521, by grants GAČR 202/07/0597, 202/08/0326 and GAAV 100100712, by PPP project of DAAD, by DFG Priority Program 1157 via GE1202/06 and the BMBF and by European ESF program NES.

-
- ¹ E. Šimánek, Phys. Lett. A **154**, 309 (1991).
 - ² J.-M. Duan and E. Šimánek, Phys. Lett. A **190**, 118 (1992).
 - ³ E. M. Chudnovsky and A. B. Kuklov, Phys. Rev. Lett. **91**, 067004 (2003).
 - ⁴ M. W. Coffey, Phys. Rev. B **49**, 9774 (1994).
 - ⁵ H. Ullmaier, R. Zeller, and P. H. Dederichs, Phys. Lett. A **44**, 331 (1973).
 - ⁶ V. G. Kogan, L. N. Bulaevskii, P. Miranović, and L. Dobrosavljević-Grujić, Phys. Rev. B **51**, 15344 (1995).
 - ⁷ R. Kaschner and P. Ziesche, phys. stat. sol. (b) **138**, 65 (1986).
 - ⁸ R. Kaschner and P. Ziesche, Physica Scripta **38**, 414 (1988).
 - ⁹ P. Lipavský, K. Morawetz, J. Koláček, E. H. Brandt, and M. Schreiber, Phys. Rev. B **77**, 014506 (2008).
 - ¹⁰ L. D. Landau and E. M. Lifshitz, *Elasticity* (Pergamon, Oxford, 1975).
 - ¹¹ P. Lipavský, K. Morawetz, J. Koláček, and E. H. Brandt, Phys. Rev. B **76**, 052502 (2007).
 - ¹² H. F. Budd and J. Vannimenus, Phys. Rev. Lett **31**, 1218 (1973).
 - ¹³ A. Kleina and K. F. Wojciechowski, *Metal Surface Electron Physics* (Elsevier Sciences, Oxford, 1996).
 - ¹⁴ P. Lipavský, K. Morawetz, J. Koláček, J. J. Mareš, E. H. Brandt, and M. Schreiber, Phys. Rev. B **69**, 024524 (2004).
 - ¹⁵ P. Lipavský, J. Koláček, K. Morawetz, and E. H. Brandt, Phys. Rev. B **65**, 144511 (2002).
 - ¹⁶ P. Lipavský, J. Koláček, K. Morawetz, E. H. Brandt, and T. J. Yang, *Bernoulli potential in superconductors* (Springer, Berlin, 2007), Lecture Notes in Physics 733.
 - ¹⁷ P. Lipavský, K. Morawetz, J. Koláček, J. J. Mareš, E. H. Brandt, and M. Schreiber, Phys. Rev. B **71**, 024526 (2005).
 - ¹⁸ E. H. Brandt, Phys. Rev. B **71**, 014521 (2005).
 - ¹⁹ See physical properties in www.webelements.com.
 - ²⁰ The pair-able charge per Cu atoms is $-0.4335e$. In Fig. 2.16 Plakida²⁴ shows results of Cava²⁵ according to which the charge transfer $-0.03e$ from chains to planes per Cu site leads to a decrease of the critical temperature by 30 K. This corresponds to $\frac{\partial \ln T_c}{\partial \ln n} = -4.82$. From Fig. 3 of [26] we can see that the specific heat coefficient drops at the same time from 4.4 mJ/gK^2 to 3.0 mJ/gK^2 which gives $\frac{\partial \ln \gamma}{\partial \ln n} = -4.13$. This is only a rough estimate since the specific heat data include chains while we need the change in plane only.
 - ²¹ Y. M. Soifer, A. Verdyan, I. Lapsker, and J. Azoulay, Physica C **408**, 846 (2004).
 - ²² N. P. Kobelev, R. K. Nikolaev, N. I. Sidorov, and Y. M. Soifer, phys. stat. sol. (a) **127**, 355 (1991).
 - ²³ K. Suenaga and G. Oomi, J. Phys. Soc. Japan **60**, 1189 (1991).
 - ²⁴ N. M. Plakida, *High-Temperature Superconductivity* (Springer-Verlag, Berlin, 1995).
 - ²⁵ R. J. Cava, A. W. Hewat, E. A. Hewat, B. Batlogg, M. Marezio, K. M. Rabe, J. J. Krajewski, W. F. Peck, and L. W. Rupp, Physica C **165**, 419 (1990).
 - ²⁶ J. W. Loram, K. A. Mirza, J. R. Cooper, and W. Y. Liang, Phys. Rev. Lett. **71**, 1740 (1993).